Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:05 PM GMT

PDB ID	:	4KHN
Title	:	Crystal structure of the ternary complex of the D714A mutant of RB69 DNA polymerase
Authors	:	Guja, K.E.; Jacewicz, A.; Trzemecka, A.; Plochocka, D.; Yakubovskaya, E.; Bebenek, A.; Garcia-Diaz, M.
Deposited on	:	2013-04-30
Resolution	:	2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

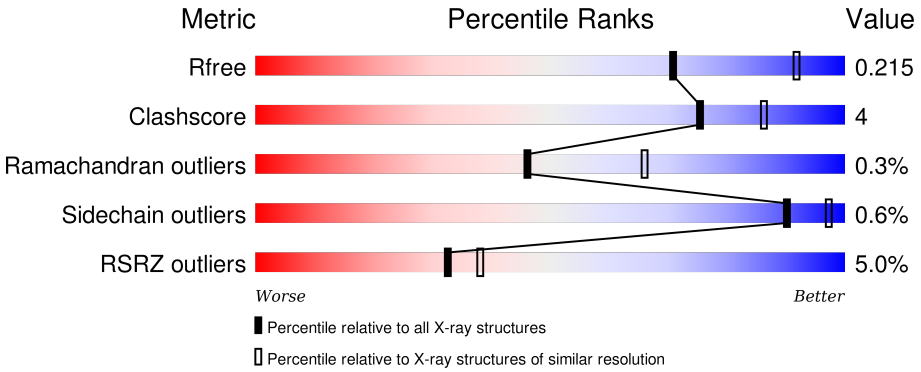
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	903	3% 92% 8%
1	B	903	7% 83% 13% •
2	C	18	6% 94% 6%
2	E	18	89% 11%
3	D	13	92% 8%

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Mol	Chain	Length	Quality of chain
3	F	13	77% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	1008	-	-	-	X
7	GOL	A	1009	-	-	-	X
8	NA	A	1010	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15657 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	901	Total	C	N	O	S	0	2	0
			7198	4640	1199	1326	33			
1	B	870	Total	C	N	O	S	0	1	0
			6730	4352	1113	1235	30			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	567	ALA	TYR	ENGINEERED MUTATION	UNP Q38087
A	714	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	567	ALA	TYR	ENGINEERED MUTATION	UNP Q38087
B	714	ALA	ASP	ENGINEERED MUTATION	UNP Q38087

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*AP*CP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			365	174	69	105	17			
2	E	18	Total	C	N	O	P	0	0	0
			365	174	69	105	17			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

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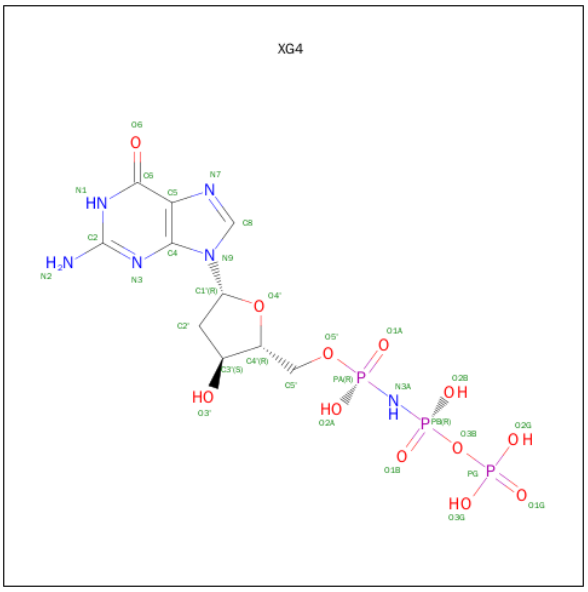
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

- Molecule 4 is 2'-DEOXY-5'-O-[(R)-HYDROXY{[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]AMINO}PHOSPHORYL]GUANOSINE (three-letter code: XG4) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

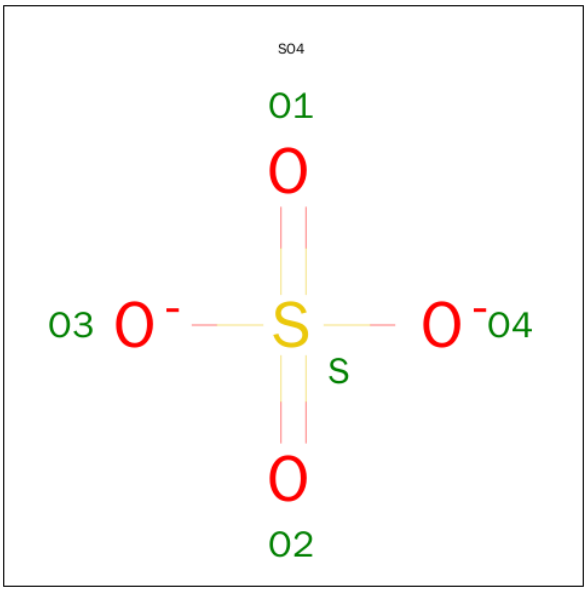


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

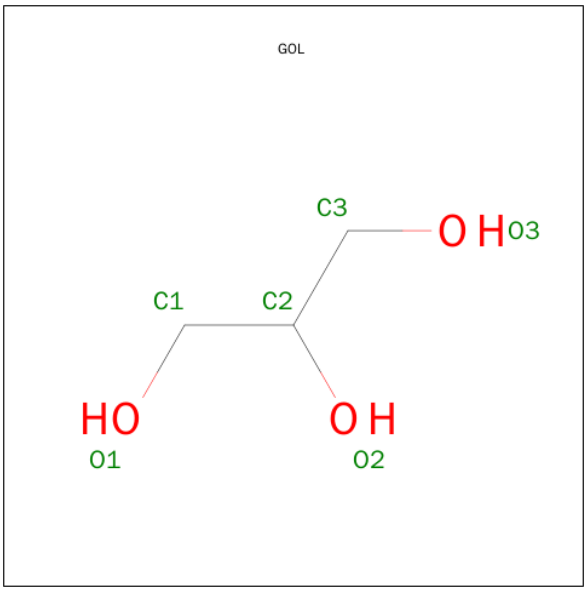
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

- Molecule 9 is water.

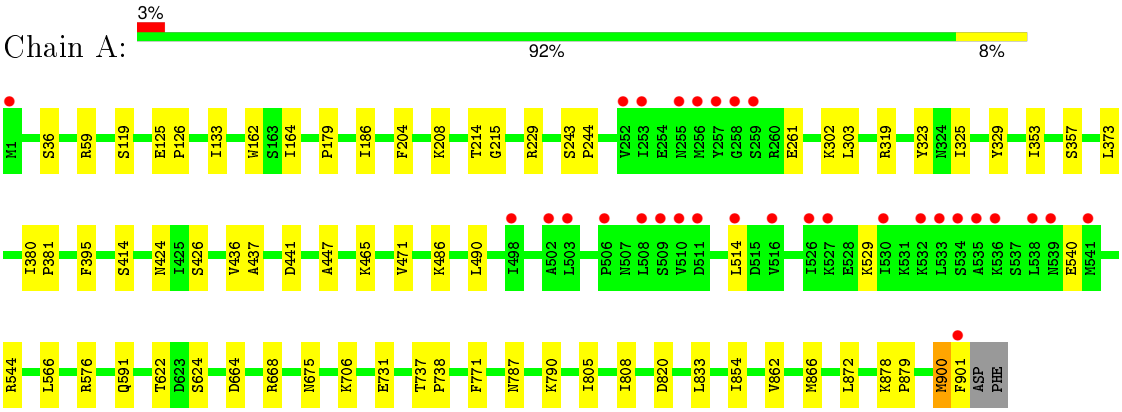
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	228	Total O 228 228	0	0
9	C	23	Total O 23 23	0	0
9	D	17	Total O 17 17	0	0
9	E	6	Total O 6 6	0	0
9	F	3	Total O 3 3	0	0
9	B	27	Total O 27 27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

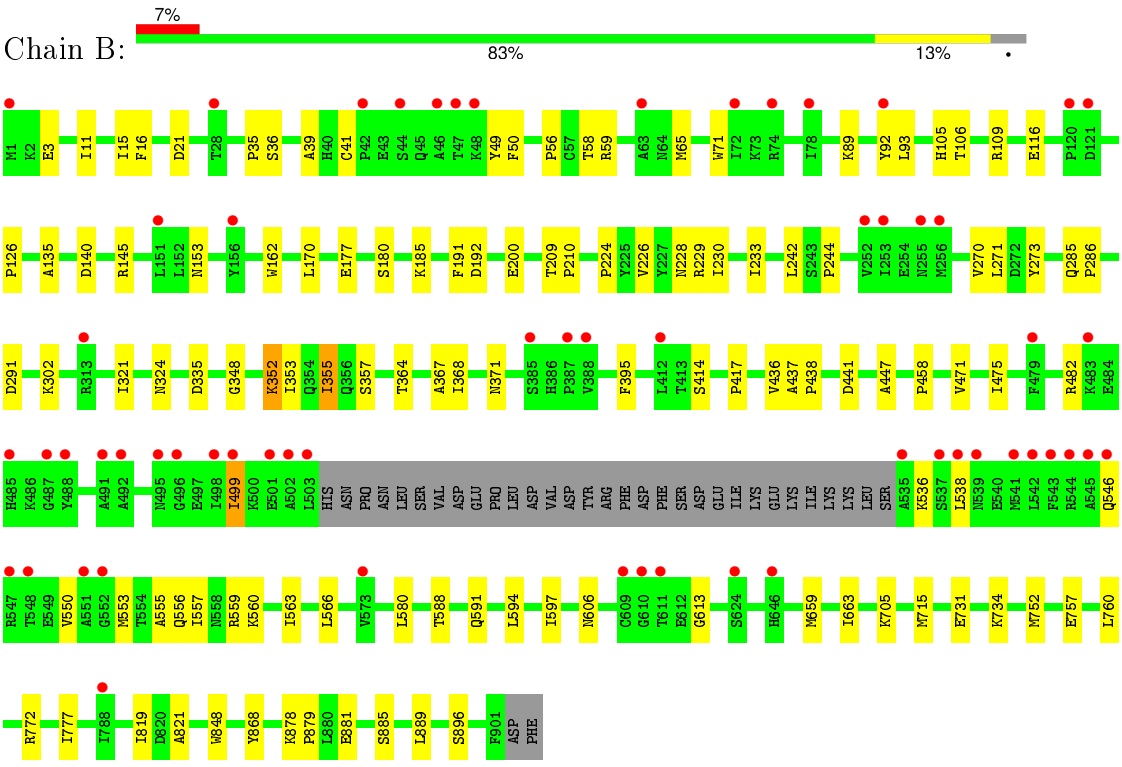
- Molecule 1: DNA polymerase

Chain A:



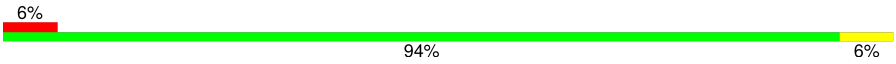
- Molecule 1: DNA polymerase

Chain B:



• Molecule 2: DNA (5'-D(*TP*CP*AP*CP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3')

Chain C:



• Molecule 2: DNA (5'-D(*TP*CP*AP*CP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3')

Chain E:

• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*C)-3')

Chain D:

• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*C)-3')

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.26Å 119.35Å 148.03Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	35.33 – 2.55 35.33 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.33-2.55) 95.5 (35.33-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1363)	Depositor
R, R_{free}	0.168 , 0.211 0.177 , 0.215	Depositor DCC
R_{free} test set	4149 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.9	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 83995 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15657	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, SO4, XG4, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.48	0/7382	0.59	1/9996 (0.0%)
1	B	0.43	0/6904	0.56	1/9388 (0.0%)
2	C	0.47	0/409	1.02	0/629
2	E	0.48	0/409	1.05	1/629 (0.2%)
3	D	0.45	0/294	1.05	1/452 (0.2%)
3	F	0.43	0/294	1.09	3/452 (0.7%)
All	All	0.46	0/15692	0.64	7/21546 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	821	ALA	C-N-CD	5.98	140.96	128.40
1	A	900	MET	CB-CG-SD	-5.85	94.86	112.40
3	F	108	DC	C1'-O4'-C4'	-5.29	104.81	110.10
2	E	18	DG	C8-N9-C4	-5.26	104.30	106.40
3	F	108	DC	O4'-C1'-N1	5.11	111.58	108.00
3	D	115	DC	C1'-O4'-C4'	-5.06	105.04	110.10
3	F	115	DC	C1'-O4'-C4'	-5.02	105.08	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7198	0	6994	38	0
1	B	6730	0	6330	72	0
2	C	365	0	203	1	0
2	E	365	0	203	1	0
3	D	263	0	148	0	0
3	F	263	0	148	1	0
4	A	31	0	13	0	0
4	B	62	0	26	2	0
4	C	31	0	13	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	25	0	0	0	0
6	B	5	0	0	0	0
7	A	12	0	16	3	0
8	A	1	0	0	0	0
9	A	228	0	0	1	0
9	B	27	0	0	0	0
9	C	23	0	0	0	0
9	D	17	0	0	0	0
9	E	6	0	0	0	0
9	F	3	0	0	0	0
All	All	15657	0	14094	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:PHE:HB2	1:B:591:GLN:HG3	1.61	0.82
1:B:560:LYS:NZ	4:B:1002:XG4:O3G	2.22	0.72
1:B:153:ASN:ND2	1:B:192:ASP:O	2.22	0.71
1:A:833:LEU:HD13	1:A:866:MET:HG2	1.73	0.70
1:A:514:LEU:HD21	1:A:529:LYS:HG2	1.74	0.69
1:B:546:GLN:HE21	1:B:550:VAL:HG23	1.59	0.68
1:A:664:ASP:OD2	1:A:668:ARG:NH1	2.26	0.68
7:A:1008:GOL:H31	4:C:101:XG4:HN3A	1.59	0.67
1:A:486:LYS:HE2	1:A:490:LEU:HD11	1.79	0.64
1:B:170:LEU:HA	1:B:177:GLU:HG3	1.80	0.63
1:A:820:ASP:N	1:A:820:ASP:OD1	2.33	0.62
1:A:668:ARG:HD2	9:A:1290:HOH:O	1.98	0.61
1:B:417:PRO:HG2	1:B:563:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1008:GOL:O3	7:A:1008:GOL:O1	2.18	0.60
1:A:395:PHE:HB2	1:A:591:GLN:HB2	1.86	0.58
1:B:475:ILE:HD12	1:B:566:LEU:HD23	1.86	0.58
1:A:303:LEU:HD21	1:A:319:ARG:HG3	1.86	0.57
1:B:35:PRO:HG3	1:B:65:MET:HG2	1.86	0.55
1:A:900:MET:HE2	1:A:901:PHE:N	2.21	0.55
1:B:36:SER:OG	1:B:59:ARG:NH1	2.39	0.55
1:B:471:VAL:HG13	1:B:566:LEU:HD21	1.88	0.54
1:B:41:CYS:HB3	1:B:58:THR:HG22	1.90	0.54
1:B:209:THR:HG21	1:B:244:PRO:HG3	1.89	0.53
1:B:606:ASN:OD1	1:B:613:GLY:N	2.42	0.53
1:A:186:ILE:HD13	1:A:325:ILE:HD13	1.91	0.53
1:B:367:ALA:O	1:B:371:ASN:ND2	2.32	0.53
1:B:109:ARG:HD2	1:B:140:ASP:OD1	2.09	0.52
1:B:15:ILE:HD13	1:B:92:TYR:CE2	2.45	0.52
1:A:303:LEU:HD23	1:A:323:TYR:HB2	1.90	0.52
1:A:36:SER:OG	1:A:59:ARG:NH1	2.42	0.51
1:B:291:ASP:OD1	1:B:302:LYS:HA	2.10	0.51
1:B:226:VAL:O	1:B:230:ILE:HG12	2.10	0.51
1:A:436:VAL:HG12	1:A:437:ALA:O	2.10	0.51
1:B:50:PHE:HD1	1:B:56:PRO:HA	1.77	0.50
1:B:482:ARG:HB2	1:B:559:ARG:HB3	1.92	0.50
1:B:105:HIS:CE1	1:B:106:THR:HG23	2.47	0.50
1:A:465:LYS:NZ	1:A:675:ASN:OD1	2.44	0.49
1:B:145:ARG:HH11	1:B:185:LYS:HA	1.78	0.49
1:B:436:VAL:HG12	1:B:437:ALA:O	2.12	0.49
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.96	0.48
1:A:787:ASN:HB3	1:A:790:LYS:HB3	1.96	0.47
1:B:482:ARG:NE	1:B:560:LYS:HB2	2.30	0.47
1:B:50:PHE:CD1	1:B:56:PRO:HA	2.50	0.47
1:A:133:ILE:HG13	1:A:229:ARG:HG2	1.97	0.47
1:B:555:ALA:HB1	1:B:559:ARG:NH1	2.29	0.47
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.95	0.47
1:B:659:MET:O	1:B:663:ILE:HG13	2.15	0.47
1:A:540:GLU:HG3	1:A:544:ARG:HE	1.79	0.47
1:B:553:MET:O	1:B:556:GLN:HG3	2.13	0.47
1:B:731:GLU:N	1:B:731:GLU:OE1	2.44	0.47
1:B:109:ARG:HG2	1:B:210:PRO:HA	1.97	0.47
1:B:353:ILE:CD1	1:B:357:SER:HB2	2.45	0.47
4:B:1002:XG4:O2B	4:B:1002:XG4:O2G	2.33	0.46
1:A:706:LYS:HE3	2:C:7:DA:N3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:VAL:HG13	1:A:566:LEU:HD21	1.97	0.46
1:A:771:PHE:CZ	1:A:872:LEU:HB2	2.51	0.46
1:B:772:ARG:HG2	1:B:868:TYR:CG	2.51	0.46
1:B:546:GLN:NE2	1:B:550:VAL:HG23	2.27	0.45
1:B:116:GLU:HG2	1:B:324:ASN:ND2	2.31	0.45
1:B:752:MET:HG2	1:B:760:LEU:HD22	1.97	0.45
1:B:458:PRO:HG2	1:B:588:THR:HG22	1.98	0.45
1:B:438:PRO:HG2	1:B:441:ASP:OD2	2.16	0.45
1:B:777:ILE:HD13	1:B:848:TRP:HZ2	1.81	0.45
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.98	0.45
2:E:8:DA:H5"	1:B:705:LYS:HD3	1.98	0.44
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.48	0.44
1:A:353:ILE:HD12	1:A:357:SER:HB2	1.99	0.44
1:A:854:ILE:HD13	1:A:862:VAL:HG21	2.00	0.44
1:B:553:MET:O	1:B:557:ILE:HG13	2.18	0.44
1:B:499:ILE:HD12	1:B:538:LEU:HD22	1.99	0.44
1:B:39:ALA:HB2	1:B:71:TRP:HH2	1.83	0.44
1:B:597:ILE:HA	1:B:597:ILE:HD12	1.76	0.44
1:B:353:ILE:HD13	1:B:357:SER:HB2	2.00	0.43
1:B:126:PRO:HB2	1:B:224:PRO:HB2	2.00	0.43
1:B:273:TYR:OH	1:B:335:ASP:HA	2.19	0.43
1:B:499:ILE:HA	1:B:499:ILE:HD13	1.85	0.43
1:A:862:VAL:O	1:A:866:MET:HG3	2.19	0.43
1:B:49:TYR:CZ	1:B:59:ARG:HD3	2.54	0.43
1:A:179:PRO:HG2	1:A:329:TYR:CE2	2.54	0.43
1:B:878:LYS:HB3	1:B:879:PRO:HD3	2.00	0.43
1:B:757:GLU:HB2	1:B:889:LEU:HD22	2.01	0.43
1:B:352:LYS:HE3	1:B:352:LYS:HB2	1.63	0.43
1:B:881:GLU:O	1:B:885:SER:HB3	2.18	0.43
1:B:3:GLU:HG3	1:B:21:ASP:HA	2.00	0.43
3:F:113:DT:H5'	1:B:734:LYS:HG2	2.00	0.43
1:B:594:LEU:HD12	1:B:594:LEU:HA	1.86	0.43
7:A:1008:GOL:H32	4:C:101:XG4:N7	2.34	0.42
1:B:126:PRO:O	1:B:228:ASN:ND2	2.52	0.42
1:B:270:VAL:O	1:B:271:LEU:HD23	2.19	0.42
1:B:191:PHE:CZ	1:B:200:GLU:HG2	2.54	0.42
1:B:15:ILE:HD12	1:B:15:ILE:O	2.19	0.42
1:A:737:THR:HA	1:A:738:PRO:HD3	1.89	0.42
1:A:731:GLU:OE1	1:A:731:GLU:N	2.48	0.42
1:B:162:TRP:CD1	1:B:321:ILE:HB	2.55	0.42
1:A:214:THR:OG1	1:A:215:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PRO:O	1:A:576:ARG:HD3	2.20	0.42
1:B:229:ARG:O	1:B:233:ILE:HG12	2.19	0.42
1:A:878:LYS:HB3	1:A:879:PRO:HD3	2.02	0.41
1:B:89:LYS:O	1:B:93:LEU:HG	2.20	0.41
1:A:162:TRP:CH2	1:A:164:ILE:HG13	2.55	0.41
1:B:285:GLN:HA	1:B:286:PRO:HD3	1.89	0.41
1:A:125:GLU:HA	1:A:126:PRO:HD2	1.90	0.41
1:A:373:LEU:HD12	1:A:380:ILE:HG22	2.03	0.41
1:B:364:THR:O	1:B:368:ILE:HG13	2.20	0.41
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.56	0.41
1:B:226:VAL:HG12	1:B:242:LEU:HD11	2.02	0.41
1:A:302:LYS:HE2	1:A:323:TYR:CZ	2.55	0.41
1:B:555:ALA:HB1	1:B:559:ARG:HH12	1.85	0.41
1:B:580:LEU:HA	1:B:580:LEU:HD12	1.81	0.41
1:A:243:SER:HA	1:A:244:PRO:HD2	1.83	0.40
1:B:11:ILE:HB	1:B:16:PHE:CE1	2.56	0.40
1:A:805:ILE:HD13	1:A:808:ILE:HD12	2.03	0.40
1:B:715:MET:HE2	1:B:715:MET:HB2	1.98	0.40
1:B:348:GLY:HA3	1:B:355:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	901/903 (100%)	870 (97%)	28 (3%)	3 (0%)	46 66
1	B	867/903 (96%)	832 (96%)	32 (4%)	3 (0%)	46 66
All	All	1768/1806 (98%)	1702 (96%)	60 (3%)	6 (0%)	46 66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	355	ILE
1	B	414	SER
1	B	819	ILE
1	A	414	SER
1	A	622	THR
1	A	424	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	749/798 (94%)	745 (100%)	4 (0%)	92 98
1	B	663/798 (83%)	658 (99%)	5 (1%)	86 96
All	All	1412/1596 (88%)	1403 (99%)	9 (1%)	90 97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	SER
1	A	261	GLU
1	A	426	SER
1	A	624	SER
1	B	180	SER
1	B	352	LYS
1	B	499	ILE
1	B	536	LYS
1	B	896	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	B	546	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	XG4	A	1001	-	28,33,33	1.78	6 (21%)	35,52,52	1.68	8 (22%)
6	SO4	A	1003	-	4,4,4	0.16	0	6,6,6	0.13	0
6	SO4	A	1004	-	4,4,4	0.22	0	6,6,6	0.18	0
6	SO4	A	1005	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	A	1006	-	4,4,4	0.21	0	6,6,6	0.13	0
6	SO4	A	1007	-	4,4,4	0.21	0	6,6,6	0.08	0
7	GOL	A	1008	-	5,5,5	0.22	0	5,5,5	0.94	0
7	GOL	A	1009	-	5,5,5	0.36	0	5,5,5	0.31	0
4	XG4	B	1001	-	28,33,33	1.80	6 (21%)	35,52,52	1.68	7 (20%)
4	XG4	B	1002	5	28,33,33	1.70	6 (21%)	35,52,52	1.75	7 (20%)
6	SO4	B	1003	-	4,4,4	0.21	0	6,6,6	0.15	0
4	XG4	C	101	5	28,33,33	1.56	4 (14%)	35,52,52	1.93	10 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XG4	A	1001	-	-	0/13/34/34	0/3/3/3
6	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
7	GOL	A	1008	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1009	-	-	0/4/4/4	0/0/0/0
4	XG4	B	1001	-	-	0/13/34/34	0/3/3/3
4	XG4	B	1002	5	-	0/13/34/34	0/3/3/3
6	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
4	XG4	C	101	5	-	0/13/34/34	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	XG4	PB-O1B	2.09	1.48	1.46
4	B	1002	XG4	PB-O1B	2.09	1.48	1.46
4	B	1001	XG4	PA-O1A	2.14	1.48	1.46
4	B	1001	XG4	PB-O1B	2.14	1.48	1.46
4	B	1002	XG4	PB-O3B	2.20	1.61	1.59
4	A	1001	XG4	PA-O1A	2.38	1.48	1.46
4	A	1001	XG4	C5-C4	2.99	1.47	1.40
4	C	101	XG4	C5-C4	3.01	1.47	1.40
4	B	1002	XG4	C5-C4	3.07	1.47	1.40
4	B	1001	XG4	C5-C4	3.07	1.47	1.40
4	A	1001	XG4	C6-C5	3.18	1.47	1.41
4	B	1002	XG4	C6-C5	3.22	1.47	1.41
4	B	1001	XG4	C6-C5	3.50	1.48	1.41
4	C	101	XG4	PB-N3A	3.56	1.72	1.63
4	C	101	XG4	C6-C5	3.68	1.48	1.41
4	B	1002	XG4	PA-N3A	3.95	1.73	1.63
4	C	101	XG4	PA-N3A	4.00	1.73	1.63
4	B	1002	XG4	PB-N3A	4.45	1.75	1.63
4	B	1001	XG4	PB-N3A	4.58	1.75	1.63
4	A	1001	XG4	PB-N3A	4.60	1.75	1.63
4	A	1001	XG4	PA-N3A	4.63	1.75	1.63
4	B	1001	XG4	PA-N3A	4.65	1.75	1.63

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101	XG4	O1A-PA-N3A	-4.48	105.03	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	XG4	C5-C6-N1	-4.02	118.09	123.59
4	C	101	XG4	C5-C6-N1	-3.95	118.19	123.59
4	B	1002	XG4	C5-C6-N1	-3.86	118.31	123.59
4	B	1001	XG4	C5-C6-N1	-3.83	118.35	123.59
4	B	1002	XG4	C2'-C1'-N9	-3.66	105.25	114.16
4	C	101	XG4	C2'-C1'-N9	-3.57	105.48	114.16
4	B	1001	XG4	PG-O3B-PB	-3.54	120.79	132.67
4	B	1001	XG4	N3-C2-N1	-3.32	122.39	127.44
4	A	1001	XG4	N3-C2-N1	-3.18	122.60	127.44
4	C	101	XG4	C4-C5-N7	-3.13	106.60	109.48
4	B	1002	XG4	C6-C5-C4	-3.06	117.24	120.90
4	C	101	XG4	C6-C5-C4	-3.06	117.24	120.90
4	A	1001	XG4	C6-C5-C4	-3.02	117.29	120.90
4	A	1001	XG4	PG-O3B-PB	-2.99	122.63	132.67
4	B	1002	XG4	N3-C2-N1	-2.97	122.92	127.44
4	B	1001	XG4	C6-C5-C4	-2.93	117.39	120.90
4	C	101	XG4	N3-C2-N1	-2.83	123.13	127.44
4	C	101	XG4	PG-O3B-PB	-2.68	123.68	132.67
4	B	1001	XG4	C4-C5-N7	-2.57	107.12	109.48
4	B	1002	XG4	PG-O3B-PB	-2.56	124.08	132.67
4	A	1001	XG4	C4-C5-N7	-2.56	107.12	109.48
4	B	1002	XG4	C4-C5-N7	-2.53	107.15	109.48
4	C	101	XG4	O1B-PB-N3A	-2.37	108.26	111.90
4	B	1001	XG4	O1A-PA-N3A	-2.12	108.64	111.90
4	A	1001	XG4	O3G-PG-O2G	2.05	115.19	107.38
4	A	1001	XG4	C2'-C3'-C4'	2.09	107.11	102.77
4	C	101	XG4	O3G-PG-O1G	2.23	117.74	110.58
4	C	101	XG4	C6-N1-C2	4.24	121.83	115.94
4	B	1002	XG4	C6-N1-C2	4.44	122.11	115.94
4	B	1001	XG4	C6-N1-C2	4.55	122.26	115.94
4	A	1001	XG4	C6-N1-C2	4.89	122.73	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1008	GOL	3	0
4	B	1002	XG4	2	0
4	C	101	XG4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	901/903 (99%)	-0.10	30 (3%) 50 56	27, 46, 85, 118	0
1	B	870/903 (96%)	0.24	60 (6%) 20 23	44, 81, 113, 135	0
2	C	18/18 (100%)	0.08	1 (5%) 28 33	29, 44, 118, 128	0
2	E	18/18 (100%)	-0.47	0 100 100	50, 66, 118, 126	0
3	D	13/13 (100%)	0.05	0 100 100	33, 42, 109, 113	0
3	F	13/13 (100%)	-0.07	0 100 100	55, 70, 111, 118	0
All	All	1833/1868 (98%)	0.06	91 (4%) 32 38	27, 62, 109, 135	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	TYR	7.7
1	B	548	THR	7.0
1	B	543	PHE	6.2
1	A	535	ALA	6.1
1	B	542	LEU	6.1
1	B	551	ALA	5.3
1	A	538	LEU	5.2
1	B	496	GLY	5.1
1	A	259	SER	4.9
1	B	492	ALA	4.8
1	A	516	VAL	4.7
1	B	541	MET	4.5
1	A	533	LEU	4.4
1	A	256	MET	4.3
1	B	488	TYR	4.3
1	B	552	GLY	4.1
1	B	499	ILE	3.9
1	B	1	MET	3.7
1	A	255	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	72	ILE	3.7
1	B	46	ALA	3.6
1	B	388	VAL	3.5
1	A	526	ILE	3.5
2	C	1	DT	3.5
1	B	252	VAL	3.4
1	B	44	SER	3.4
1	B	624	SER	3.4
1	B	256	MET	3.4
1	B	544	ARG	3.3
1	B	42	PRO	3.3
1	A	534	SER	3.3
1	B	47	THR	3.3
1	B	538	LEU	3.2
1	A	508	LEU	3.2
1	B	545	ALA	3.1
1	B	498	ILE	3.1
1	B	74	ARG	3.0
1	B	547	ARG	3.0
1	B	479	PHE	3.0
1	A	252	VAL	3.0
1	A	1	MET	2.9
1	B	502	ALA	2.9
1	B	491	ALA	2.8
1	B	546	GLN	2.7
1	A	503	LEU	2.7
1	B	537	SER	2.7
1	B	539	ASN	2.7
1	A	498	ILE	2.6
1	B	387	PRO	2.6
1	B	483	LYS	2.6
1	B	501	GLU	2.6
1	A	530	ILE	2.6
1	A	510	VAL	2.5
1	A	541	MET	2.5
1	A	539	ASN	2.5
1	B	48	LYS	2.5
1	B	151	LEU	2.5
1	B	156	TYR	2.5
1	B	503	LEU	2.5
1	B	646	HIS	2.5
1	A	509	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	535	ALA	2.4
1	B	253	ILE	2.4
1	A	514	LEU	2.4
1	B	609	CYS	2.4
1	A	506	PRO	2.4
1	B	487	GLY	2.3
1	B	412	LEU	2.3
1	A	502	ALA	2.3
1	B	495	ASN	2.3
1	B	611	THR	2.3
1	B	63	ALA	2.3
1	A	536	LYS	2.2
1	A	527	LYS	2.2
1	B	385	SER	2.2
1	B	485	HIS	2.2
1	B	573	VAL	2.2
1	B	610	GLY	2.2
1	B	28	THR	2.2
1	A	901	PHE	2.1
1	A	511	ASP	2.1
1	B	121	ASP	2.1
1	A	532	LYS	2.1
1	B	120	PRO	2.1
1	B	313	ARG	2.1
1	B	255	ASN	2.0
1	A	253	ILE	2.0
1	A	258	GLY	2.0
1	B	78	ILE	2.0
1	B	788	ILE	2.0
1	B	92	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	GOL	A	1009	6/6	0.84	0.25	3.72	66,73,73,73	0
7	GOL	A	1008	6/6	0.90	0.25	2.78	44,50,62,69	0
8	NA	A	1010	1/1	0.95	0.21	2.61	46,46,46,46	0
4	XG4	C	101	31/31	0.97	0.21	0.99	19,31,68,136	0
6	SO4	A	1007	5/5	0.89	0.17	0.90	136,137,137,139	0
4	XG4	A	1001	31/31	0.96	0.14	0.21	37,58,206,206	0
6	SO4	A	1004	5/5	0.94	0.15	0.09	94,95,96,103	0
4	XG4	B	1002	31/31	0.93	0.19	0.06	47,59,112,307	0
4	XG4	B	1001	31/31	0.88	0.16	-0.41	68,100,242,271	0
6	SO4	A	1003	5/5	0.99	0.14	-0.73	47,47,48,53	0
6	SO4	B	1003	5/5	0.94	0.14	-3.39	93,95,98,98	0
5	CA	A	1002	1/1	1.00	0.22	-	42,42,42,42	0
6	SO4	A	1005	5/5	0.91	0.11	-	114,116,118,118	0
5	CA	B	1004	1/1	0.97	0.31	-	82,82,82,82	0
6	SO4	A	1006	5/5	0.94	0.19	-	109,110,111,113	0

6.5 Other polymers

There are no such residues in this entry.